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Numerical Simulation of Gaseous Flow in Microchannel

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Abstract : A numerical simulation on nitrogen gas flow in a long parallel plate microchannel was performed to obtain the effect of compressibility and rarefaction on gaseous flow in microchannels. The simulation was based on steady, two dimensional compressible Navier-Stokes and energy equations with noslip and first order slip boundary conditions. The channel was 1.2 μm deep and 3000 μm long. The Reynolds numbers were in the range of order from 10^{-2} to 10^{-1}. So the flow was assumed to be laminar. The computations were performed on various pressure ratios. The outlet pressure was fixed to atmospheric pressure. The outlet Knudsen number was 0.0585, consequently the flow was in the slip flow regime. The computations were performed with the assumption of isothermal channel walls. The results were compared with the experimental data. The agreement was good.

Key words : Knudsen number, Mean free path, Rarefaction effect, Compressibility.

Introduction

Micromachining technology is an exciting field today. Micron size mechanical devices are encountered in a widening field of disciplines. Micro-Electro-Mechanical System (MEMS) refers to devices that have a characteristic length of less than 1 mm but more than 1 μm[1], and combines electrical and mechanical components. MEMS applications range from consumer products to industrial tools, biomedical micro-devices and instrumentation. A systematic research in micromechanical devices started in the late 1980's. Manufacturing process that can create MEMS devices has been developed in recent years. Micro-pumps, micro-nozzles, micro-turbines, micro-valves, micro-motors, micro-actuators, micro-accelerometers, micro-heat-exchangers, micro-reactors, are some of the examples of micro-devices. In order to design such microsystems effectively it is necessary to understand the physical laws governing the flows in micro-conduits. The characteristic length scale that governs the energy and momentum transfer between MEMS and their environments is typically on the order of microns. Experimental investigation with these micro-geometries

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is very difficult due to their size. Therefore numerical analysis is an alternative to investigate the flow in micro-geometries.

Many experimental[1]-[4] and numerical[5]-[7] studies indicate that remarkable differences and conflicts exist in the micro-channel flow and heat transfer characteristics compared with those in conventional size channels. Choi et al[8] found that the friction coefficient for laminar nitrogen gas flow in micro-tubes having diameters smaller than 10 μm was about 53, which is lower than the conventional value of 64. But Wu and Little[9] reported that the friction coefficient for rough microchannel flow was much higher than 64. Pong and Ho[3] investigated pressure distribution in microchannels and found that the distribution was not linear and compressibility was an important feature in a microchannel. Harley et al[2] conducted analytical and experimental investigations on gaseous flow in a (2-D) microchannel. That study demonstrated the existence of nonzero wall velocity and showed the contribution of slip on the mass flow and pressure drop. The work of van den Berg et al[10] is a (1-D) perturbation analysis of radially symmetric flow without considering slip flow effect. This study reported the existence of non-constant pressure gradient and showed the effect of compressibility. Karniadakis[11] extended the classical Maxwell/Smoluchowski slip conditions by including higher order Knudsen number effect to simulate heat and momentum transfer in microflows. A rigorous investigation of microflows was performed by Arkilic at el[1]. They presented a (2-D) analysis with a first order velocity slip boundary condition, demonstrating the effect of both compressibility and rarefaction in long microchannels. Through perturbation analysis of the full compressible (2-D) Navier-Stokes equations in Cartesian coordinates, it was shown that the zero order analytic solution corresponds well with experimental results of Pong et al[3].

Nomenclature

a	speed of sound [m/s]
f	Darcy friction factor
H	channel height [m]
Kn	Knudsen number
n	normal coordinate on the channel wall [m]
R	gas constant [J/kg.K]
Re	Reynolds number
u, v	velocity components [m/s]
$\bar{u}$	crosswise average velocity [m/s]
x, y	components of coordinate [m]

Greek symbols

λ	mean free path [m]
μ	dynamic viscosity [$N.s/m^2$]
μm	micrometer
ρ	density [kg/m^3]
σ_T	energy accommodation coefficient
σ_m	momentum accommodation coefficient
τ	shear stress [pa]

Subscript

1	channel inlet
2	channel outlet

In spite of a large number of works so far, many parts of the physical laws governing the fluid flow and heat transfer in microgeometries remain unknown[12]. The objective of this study is to investigate the gaseous flow characteristics in a microchannel. Pressure drop of nitrogen flow in a parallel plate were investigated numerically. Mass flow rate and friction factor behavior were also investigated.

2. Model development

2.1 Problem statement

We considered two dimensional nitrogen gas flow between two long parallel flat plates. Figure 1 shows the geometry of the microchannel. The length and height of the channel were 3000 and 1.2 μm respectively. We used five pressure ratios 1.34, 1.68, 2.02, 2.361 and 2.701. The inlet and wall temperature was 314°K. Table1 shows the properties of the working fluid nitrogen. The outlet pressure was fixed at atmospheric pressure, 100.8 kPa. The microchannel characteristic length was in the range of 1-100 μm.

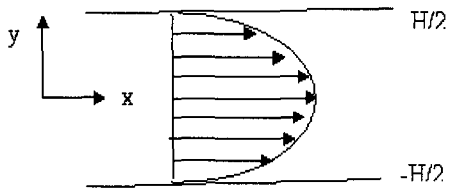

Fig. 1 Schematic diagram of the parallel plate channel

So rarefaction effect can not be neglected. Also, the flow is pressure driven and characteristic length is small compared to the length of the channel (i.e. L≫H), so the pressure gradient is high. Therefore compressibility is significant though the Reynolds number is low[1],[5].

2.2 Governing equations

It is known that the Navier-Stokes equations are the first order approximation of the Chapman-Enskog solution and can be extended to the slip flow region with the Maxwell's slip boundary condition. We assumed the flow to be steady, laminar, compressible and two-dimensional. To compare mass flow rate data with the analytical data by Arkilic et. al.[1], we considered 3D channel where width W is 40.0 μm. As the aspect ratio (width/height) is very high (33.33), the flow variation in the z-direction can be assumed to be negligible.

Table 1 Physical constants of nitrogen

Parameters	Value
Absolute viscosity μ	1.85×10^{-5} (N-s/m^2)
Specific gas constant R	296.7 (J/kg-°K)
Ratio of specific heats γ	1.4

The continuity equation is given by

$$\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}=0 \tag{1}$$

The momentum equations

$$\rho\left(u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right)=-\frac{\partial p}{\partial x}+ \mu\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{1}{3}\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 v}{\partial x\partial y}\right)\right] \tag{2}$$

$$\rho\left(u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)=-\frac{\partial p}{\partial y}+ \mu\left[\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{1}{3}\left(\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 u}{\partial x\partial y}\right)\right] \tag{3}$$

$$\rho c_p\left[u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}\right]=\left[u\frac{\partial p}{\partial x}+\frac{\partial p}{\partial y}\right]+k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)+ \quad (4)$$
$$\mu\left[2\left(\frac{\partial u}{\partial x}\right)^2+2\left(\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)^2-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)^2\right]$$

The equation of state for ideal gas

$$p=\rho RT \quad (5)$$

We used Stoke's hypothesis $\lambda+\frac{2}{3}\mu=0$, in momentum and energy equations which relates to the first and second kind of viscosity[14].

The ratio of the mean free path $\lambda=\frac{\mu\sqrt{\pi}}{\rho\sqrt{2RT}}$ and the characteristic length H is known as the Knudsen number $Kn=\frac{\lambda}{H}$. The different Knudsen number regimes are determined empirically and are therefore only approximate for particular flow geometry. In the zero Knudsen number, the transport terms in the continuum and energy equations are negligible and the Navier-Stokes equations then reduce to the inviscid Euler equations. Gas microflow can be classified into four regions according to its Knudsen numbers. The flow is considered continuum for $Kn<10^{-3}$, slip flow for $10^{-3}<Kn<10^{-1}$, transition flow for $10^{-1}<Kn<10$, and free molecule flow for $Kn>10$. We normalized the variables as follows:

Velocities were normalized by the speed of sound $a=\sqrt{\gamma RT}$. The streamwise coordinate x was normalized by the channel length L, the wall normal coordinate by the channel height H, temperature T, density ρ and pressure p by the inlet temperature T_1, inlet density ρ_1 and inlet dynamic pressure $\rho_1 a_1^2$ respectively. Reynolds number is defined by $Re=\frac{\bar{\rho}\bar{u}D_h}{\mu}$, where $\bar{\rho}$ and $\bar{u}$ are the cross sectional average density and velocity and $D_h=2H$ is the hydraulic diameter of the channel. Mach number is defined by $Ma=\frac{\bar{u}}{a}$.

3. Boundary conditions

3.1 Slip wall boundary conditions

We assumed the flow steady state and isothermal. The slip velocity boundary condition was proposed by Maxwell for an isothermal flow[14],[15]:

$$u_{gas}-u_{wall}=\frac{2-\sigma_m}{\sigma_m}Kn\frac{\partial u_s}{\partial n} \quad (6)$$

and the temperature jump boundary condition by Von Smoluchowski as

$$T_{gas}-T_w=\frac{2-\sigma_T}{\sigma_T}\left[\frac{2\gamma}{\gamma+1}\right]\frac{Kn}{Pr}\frac{\partial T}{\partial n} \quad (7)$$

Where $\left(\frac{\partial u_s}{\partial n}\right)$ and $\left(\frac{\partial T}{\partial n}\right)$ shows the variation of tangential velocity and temperature normal to the wall. The slip conditions expressed in (6) and (7) are in normalized form. The coefficients σ_m and σ_T are the tangential momentum and energy accommodation coefficients respectively. These two coefficients reflect the nature of tangential momentum and energy transfer between the impinging gas molecules and the solid wall. If the surface is smooth on the molecular length scale of the incident gas particles, the reflection will be specular where $\sigma_m = 0$, on the other hand if the surface is rough on the molecular length scale of the gas particles, the reflection will be diffuse where $\sigma_m = 1$[16]. It is assumed that (1- σ_m) of the molecules are reflected specularly and σ_m of the molecules are reflected diffusely from the wall[17]. In the present study we considered $\sigma_m = 1$ and $\sigma_T = 1$.

3.2 Noslip boundary conditions

We considered uniform inlet velocity. The pressure boundary conditions were used at the inlet and outlet boundaries. Noslip boundary conditions were imposed on the walls. The inlet gas temperature and the wall temperature were fixed to 314°K.

3.3 Numerical solutions

The governing equations along with appropriate boundary conditions were solved by finite volume method employing SIMPLE algorithm. The Quick scheme was implied for the nonlinear convective terms. Convergence criterion was set as normalized residual to 10^{-8} for energy equation and 10^{-6} for all other equations.

Table 2 Grid independency test

Grid	x=0.0005m	x=0.0015m	x=0.0025m
9×2000	0.471066	0.578688	0.815329
13×4000	0.471223	0.578874	0.815021

To evaluate the grid size effect grid independency tests were carried out. The cross sectional velocities at x=0.00297m for two different sizes of grid 9×2000 and 13×3000 were evaluated and compared. The difference of velocities is about 0.03%. For convenience grid size 13×3000 was used for the present study.

4. Results and discussion

We simulated nitrogen flow in a parallel plate channel. For validation, the simulation results were compared with the experimental results. Normalized slip flow pressure distribution in the streamwise direction is compared with the experimental result[3] in Fig.2.

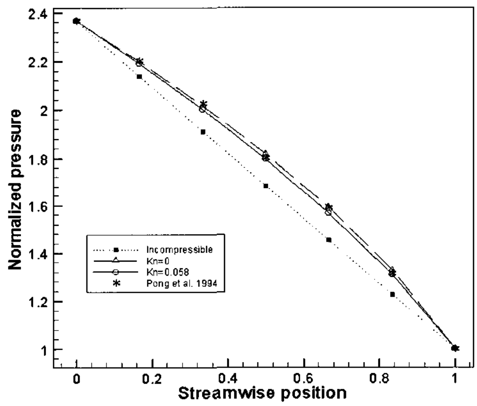

Fig. 2 Absolute pressure of nitrogen flow depicted as a function of x/L, normalized with the outlet pressure.

The agreement is good. Pressure distribution for incompressible and compressible flow with noslip boundary condition are also shown. It can be predicted from the figure that in the microchannel flow the pressure distribution is nonlinear and pressure nonlinearity in the case of noslip (Kn=0) flow is higher than that of slip flow.

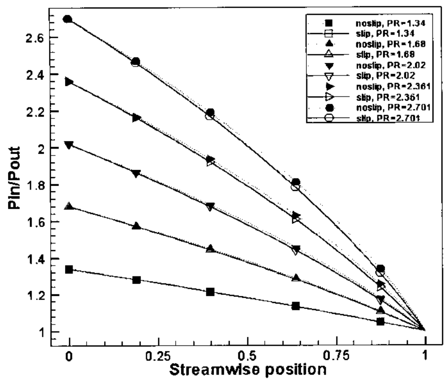

Fig. 3 Normalized pressure distribution of nitrogen flow with slip and noslip boundary conditions as a function of x/L, Kn=0.058.

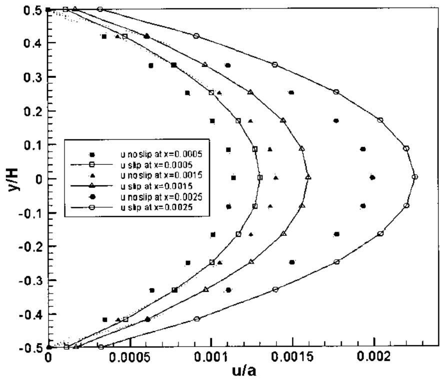

Fig. 4 Streamwise slip and noslip velocity distribution at different locations on x-axis.

Figure 3 shows the normalized pressure distribution of slip and noslip flows at different pressure ratios. The pressures are normalized with the outlet pressure. It is clear from the figure that though the Mach numbers were low in the range of order from 10^{-4} to 10^{-3}, nonlinearity is significant. When the pressure ratio is higher then the pressure nonlinearity is also higher. The deviation of nonlinearity increases as with the distance to the streamwise position. At the low pressure ratio the slip and noslip pressure distributions are nearly the same i.e. the flow behaves like incompressible flow.

Figure 4 represents the mean cross sectional velocity distribution subject to the slip and noslip boundary conditions.

The velocities were taken at x=0.0005, x=0.0015 and x=0.0025m and were normalized with the speed of sound. Pressure ratio was fixed to 2.701 to evaluate the slip effect. We see that in all the cases the slip velocities are higher than their noslip counterparts. In all the cases the velocities increase with the distance form the inlet.

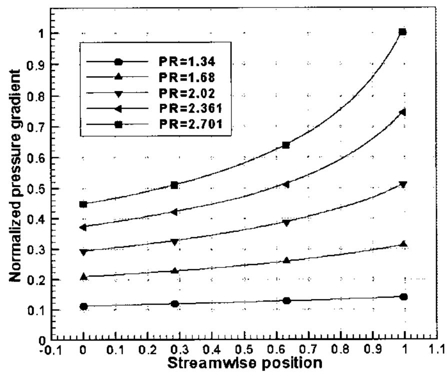

Fig. 5 Normalized pressure gradient distribution as a function of x/L.

Normalized pressure gradients are depicted by the Fig. 5. When the pressure ratio is small then pressure gradient is nearly constant. The pressure gradient increases with increasing pressure ratios. The rate of increase of pressure gradient is small near the inlet but it increases rapidly near the outlet. Normalized density and Knudsen numbers are depicted in Fig. 6. The flow variables were normalized with the corresponding outlet values.

In Fig.5 it has already been shown that the rate of increase of pressure gradient near the outlet of the channel is higher. By the ideal gas law, density is proportional to pressure, so density decreases from inlet towards outlet. Knudsen number increases toward the outlet.

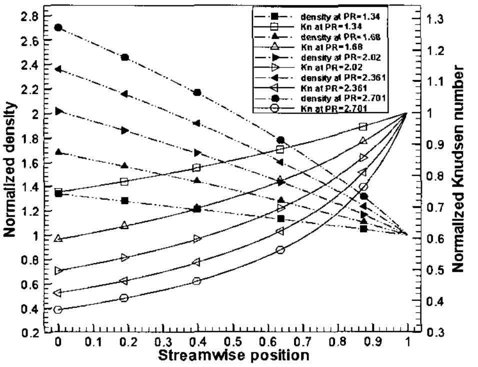

Fig. 6 Normalized pressure and Knudsen number distribution in the streamwise direction.

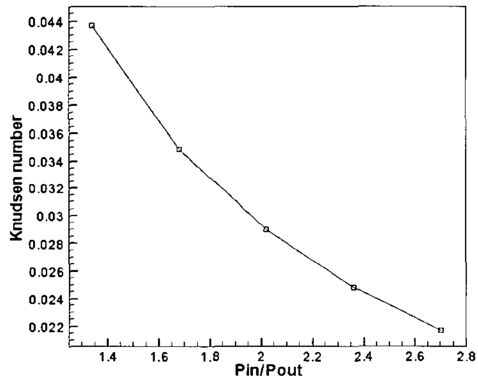

Fig. 7 Correlation between inlet Knudsen numbers and pressure ratios.

Figure 6 represents that the higher the density, the lower the Knudsen number.

Figure 7 shows the correlation between Knudsen numbers and pressure ratios.

The mass flow rates of slip and noslip flow models are presented by the Fig.8. The analytical mass flow rate defined by[1]

$$m = \frac{H^3 p_2^2 w}{24\mu LRT}\left[PR^2 - 1 + 12\left(\frac{2-\sigma_m}{\sigma_m}\right)Kn_2(PR-1)\right]$$

agrees well with our calculation. It is clear from the Fig.8 that the mass flow rate of slip model is higher than that of noslip model. It is due to lower friction factor in the case of slip flow model. Average Darcy friction factors of slip and noslip models are displayed as the function of pressure ratios in Fig.9.

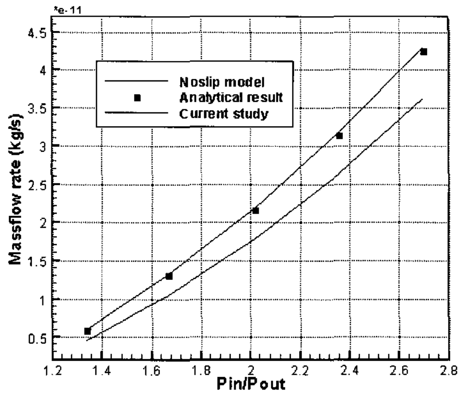

Fig. 8 Mass flow rate of slip and noslip model as a function of pressure ratios.

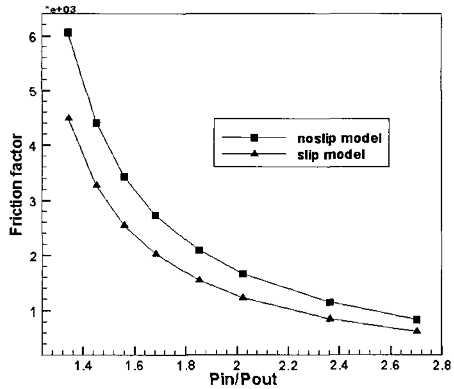

Fig. 9 Friction factors of slip and noslip model are depicted as the function of pressure ratios.

Friction factor is higher at low pressure ratios and it decreases with the increase of pressure ratios. When the pressure ratio is the highest the friction factor is the lowest. This reduction is due to the increase of velocity.

Darcy friction factor is defined as $f_D = \frac{8\tau_w}{\rho(\bar{u})^2}$. When pressure ratio increases then shear stresses also increase but friction factor is inversely proportional to the square of the cross sectional average velocity $\bar{u}$. So the influence of average velocity is large and the friction factor decreases.

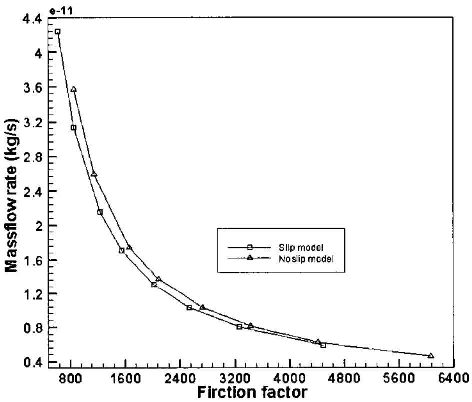

Fig. 10 Mass flow rate of slip and noslip model as a function of friction factor.

The correlation between friction factors and mass rates are depicted in Fig. 10. It shows the lower mass flow rate at the higher friction factor and the mass flow rate decreases with the increase of friction factor. This is because when the friction factor increases then the velocity and consequently the mass flow rate decreases.

We evaluated friction coefficients (fRe) for different pressure ratios. For pressure ratio 1.34 and 2.701 the corresponding friction coefficients are 71.051 and 71.058 respectively. Therefore the effect of pressure ratio on friction coefficient is negligible. The value of friction coefficient for conventional parallel plate channel is 96[18] which is much higher than the friction coefficient evaluated by the slip model.

5. Conclusion

Two dimensional compressible Navier Stokes momentum and energy equations were solved in a parallel-plate microchannel. The following conclusions can be made:

There is significant effect of compressibility and rarefaction in microchannel flow. The friction coefficient of slip flow model in the parallel-plate is lower than the conventional value of 96. Even though the pressure gradient in the microchannel is extremely high but the velocity may be low.

Acknowledgement

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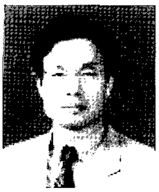
Author Profile



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